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# International Research Center for Elements Science – Synthetic Organotransformation –

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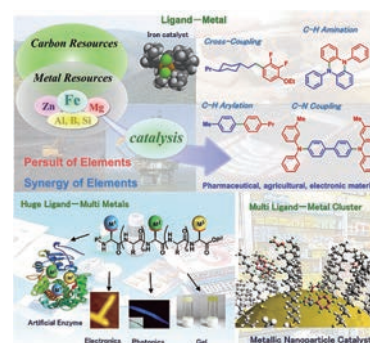
University of St Andrews, U.K., 13 June–6 August  
University of Bristol, U.K., 19 June–21 August

## Guest Scholar

HAJRA, Alakananda (D Eng) Visva-Bharati University, India, 1 July–14 August

## Scope of Research

Our research activity focuses on the development of new molecular transformations, which can contribute to better or ideal synthesis of functional molecules as well as to exploitation of new chemical (metal and carbon) resources. The present research subjects are (1) metal-catalyzed carbon–carbon and carbon–heteroatom bond forming reactions by using universal metals such as iron (2) development of smart materials based on synergistic effect of various metals on artificial peptides (3) development of smart metallic nanoparticle catalysts based on supramolecular approaches (4) understanding of reaction mechanism of these catalytic reactions with the help of quantum chemical methods and synchrotron X-ray absorption spectroscopy.



## KEYWORDS

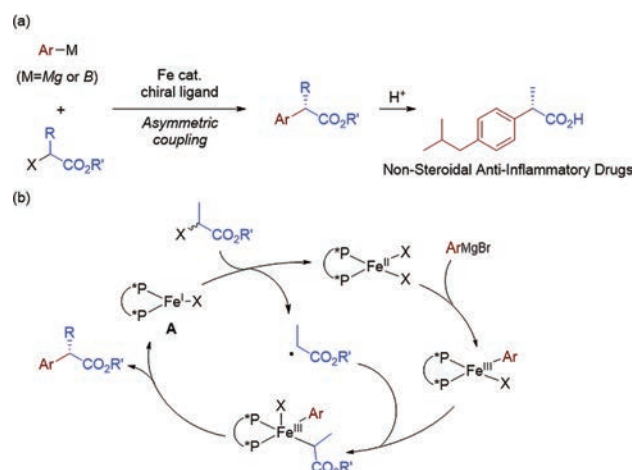
Selective Organic Reaction      Iron Catalyst      Metalated Peptide Catalyst  
Metallic Nanoparticle Catalyst      Solution-Phase XAS Analysis

## Selected Publications

Sugimoto, K.; Takaya, H.; Maekawa, M.; Kuroda-Sowa, T., Controlled Self-Assembly of a 2-D Sheet Coordination Polymer and Monomer Containing an Eight-Membered Cu<sub>4</sub>I<sub>4</sub> Crown Motif, *Cryst. Growth. Des.*, **18**, 571-575 (2018).  
Hirano, M.; Sano, K.; Kanazawa, Y.; Komine, N.; Maeno, Z.; Mitsudome, T.; Takaya, H., Mechanistic Insights on Pd&sol;Cu-Catalyzed Dehydrogenative Coupling of Dimethyl Phthalate, *ACS Catal.*, **8**, 5827-5841 (2018).  
Isozaki, K.; Shimoaka, T.; Oshiro, S.; Yamaguchi, A.; Pincella, F.; Ueno, R.; Hasegawa, T.; Watanabe, T.; Takaya, H.; Nakamura, M., Robust Surface Plasmon Resonance Chips for Repetitive and Accurate Analysis of Lignin–Peptide Interactions, *ACS Omega*, **3**, 7483-7493 (2018).

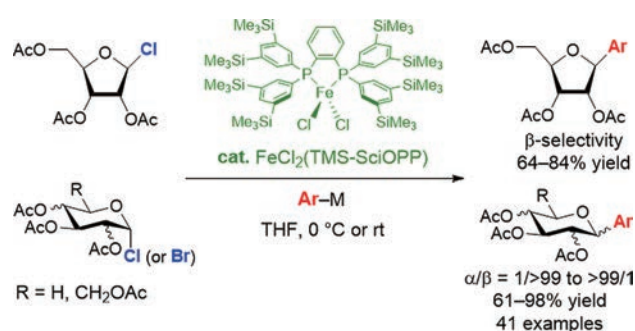
## Iron-Catalyzed Cross-Coupling Reactions

Transition-metal-catalyzed carbon–carbon and carbon–heteroatom bond forming reactions are powerful tools for the synthesis of functional molecules. Our group focuses on use of iron as a catalyst, and so far developed a variety of iron-catalyzed cross-coupling reactions, some of which can't be achieved by conventional transition-metal catalysts such as palladium. As recent representative examples, we developed the first example of iron-catalyzed enantioselective cross-coupling reaction of alkyl halides, which enable facile access to optically active products from readily available racemic halides (Figure 1a). By using DFT and AFIR calculations, we revealed that the reaction proceeds via a novel  $\text{Fe}^{\text{I-III}}$  mechanism (Figure 1b).



**Figure 1.** (a) Enantioconvergent coupling of alkyl halides and (b) its mechanism by theoretical calculation.

Moreover, we developed diastereoselective iron-catalyzed cross-coupling reaction of various glycosyl halides with aryl metal reagents for the efficient synthesis of aryl C-glycosides, which are of significant pharmaceutical interest due to their biological activities and resistance toward metabolic degradation (Figure 2).



**Figure 2.** Synthesis of Aryl C-Glycosides via Iron-Catalyzed Cross Coupling of Halosugars.

## Novel Transition-Metal Catalyst Bound with Functional Amino Acid or Peptide

This project focuses on the development of smart materials based on the synergistic effect of various metals on artificial peptides. Based on this concept, we have developed novel ruthenium complex bound with norvaline, which catalyzes efficient and selective oxidation of several methoxy-benzene analogues to quinones. Now we are trying further modifications of the catalysts toward the investigation of future chemical resources.

## Supramolecular Approach for Creating Enhanced Catalysis of Metallic Nanoparticles

This project focuses on the development of highly active and selective metallic nanoparticle and cluster catalysts. To achieve this purpose, four key methodologies have been developed: 1) creation of reaction field with advanced self-assembly, 2) design of selective molecular transformation with multi-points intermolecular interaction, 3) size selective synthesis of metallic nanoparticles and clusters, and 4) utilization of plasmonic resonance with light.

